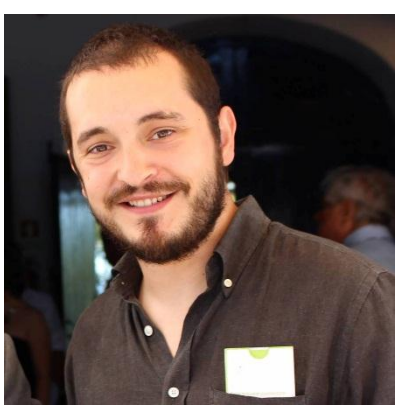
BioISI - Biosystems & Integrative Sciences Institute

BioISI Research Seminar

pH: a tricky, yet important property to deal with in molecular simulations



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BioISI/FCUL

Host: Miguel Machuqueiro (CBS-BioISI)

When: Thursday March - 12h00
Where: Building C2, Room 2.4.16

The role of pH is crucial in most biochemical processes. All living systems spent a significant fraction of its energy to control the pH value of their cellular compartments. For example, the electron transport chain could not work without proton (un)binding events. However, in biomolecular simulations, it is very tricky to control this property since bond breaking (formation) is not easily described by classical methods such as molecular dynamics (MD). In this talk, I will introduce the constant-pH molecular dynamics simulations (CpHMD) method that has been developed in our group over the last decade. In CpHMD, the conformational space of (bio)molecules is sampled using a MD simulation that is periodically interrupted to allow protonation states changes depending on the pH and conformation. With this method, we can simulate any molecule with titrable groups at a user-defined pH value, similar to a typical wet-lab experiment. In fact, CpHMD was already successfully applied to small peptides (such as kyotorphin or glutathione), proteins (prion protein or beta 2-microglobulin) and membranes (containing anionic lipids). I will show some application examples of this methodology and, hopefully, help to establish bridges and triggering new collaborations with current BioISI groups.

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